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Modelling Catalytic Structures with Python and ASE

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ABSTRACT

Voltaic cells hold great potential as a source of clean electricity generation. These fuel sources are more efficient than combustion engines, and they do not produce environmentally harmful by-products. The electrochemical reaction which occurs within the cell is typically catalyzed by platinum, which increases the cost. The search for a better performing, less expensive catalyst is hindered by the lack of a complete, predictive theory of catalysis. Using Quantum Espresso and the Atomic Simulation Environment library for Python, we created a tool for nanoHUB.org which can visually and computationally model catalytic surfaces. This tool can simulate nanoparticles and metallic surfaces over a metallic bulk. It provides a visual of the input structure and generates an input file for use with Quantum Espresso's plane-wave self-consistent field calculation. The user can also run the Quantum Espresso calculation and the tool will automatically calculate the surface and adsorption energies. This should provide an easier method to study catalysts than lab work, and the inclusion of a visual component allows for the analysis of geometric properties.

KEYWORDS

computational catalysis, simulation, chemistry, electrochemical, oxygen reduction reaction, oxygen evolution reaction, density functional theory